

chain nodes :

15

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 16

chain bonds :

14-15

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-16 5-6 5-13 7-8 7-12 8-9 9-10 9-13
10-11 10-14 11-12 14-16

exact/norm bonds :

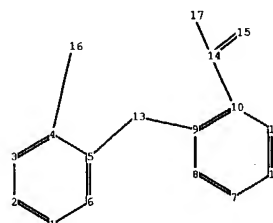
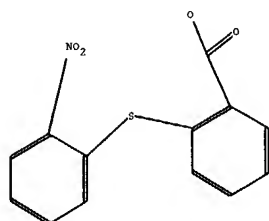
4-16 5-13 9-13 10-14 14-15 14-16

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:Atom



chain nodes :

13 15 16 17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

ring/chain nodes :

14

chain bonds :

4-16 5-13 9-13 14-15 14-17

ring/chain bonds :

10-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

5-13 9-13 10-14 14-15 14-17

exact bonds :

4-16

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom

10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:Atom

17:CLASS

10/030,251

=> d his

(FILE 'HOME' ENTERED AT 14:35:10 ON 23 SEP 2003)

FILE 'REGISTRY' ENTERED AT 14:35:16 ON 23 SEP 2003

L1 STRUCTURE UPLOADED
L2 QUE L1
L3 4 S L2
L4 1160 S 3068.74/RID
L5 SCREEN 2076
L6 STRUCTURE UPLOADED
L7 QUE L6 AND L5
L8 2 S L7
L9 112 S L2 SSS FUL
L10 37 S L7 SSS FUL

FILE 'CAPLUS' ENTERED AT 14:45:23 ON 23 SEP 2003

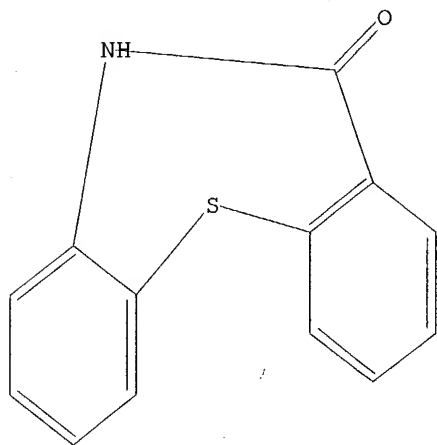
L11 88 S L9
L12 44 S L10
L13 13 S L11 AND L12

FILE 'REGISTRY' ENTERED AT 14:46:04 ON 23 SEP 2003

=> d l2

L2 HAS NO ANSWERS

L1 STR



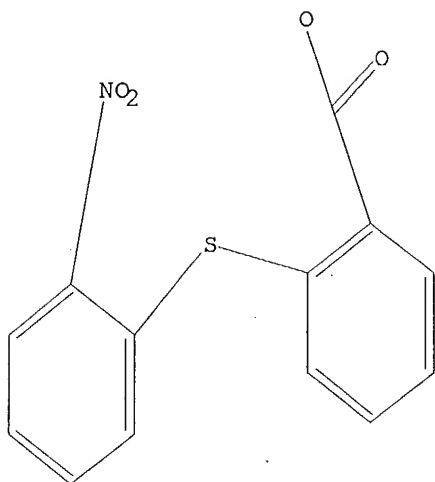
Structure attributes must be viewed using STN Express query preparation.
L2 QUE ABB=ON PIU=ON L1

=> d l7

L7 HAS NO ANSWERS

L5 SCR 2076
L6 STR

10/030,251



Structure attributes must be viewed using STN Express query preparation.
L7 QUE ABB=ON PLU=ON L6 AND L5

=> d ibib abs hitstr l13 1-13

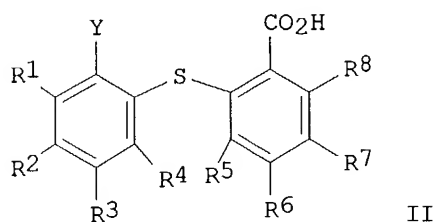
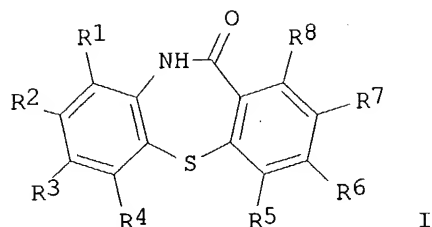
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

10/030,251

applicant

L13 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:463259 CAPLUS
DOCUMENT NUMBER: 131:102294
TITLE: Preparation of dibenzothiazepines and their intermediates
INVENTOR(S): Harada, Katsumasa; Nishino, Shigehide; Yoshii, Kiyotaka
PATENT ASSIGNEE(S): Ube Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11199574	A2	19990727	JP 1998-15022	19980109
WO 2001004106	A1	20010118	WO 1999-JP3719	19990709
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9946506	A1	20010130	AU 1999-46506	19990709
EP 1201663	A1	20020502	EP 1999-929773	19990709
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
EE 200200014	A	20030415	EE 2002-14	19990709
NO 2002000059	A	20020304	NO 2002-59	20020107
PRIORITY APPLN. INFO.:			JP 1998-15022	A 19980109
			WO 1999-JP3719	A 19990709
OTHER SOURCE(S):		CASREACT 131:102294; MARPAT 131:102294		
GI				



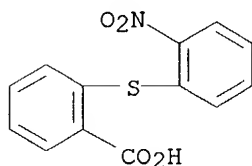
AB Dibenzothiazepines I [R1-R8 = H, (substituted) alkyl, alkoxy, alkylcarbonyl, aryl, aryloxy, arylcarbonyl], useful as intermediates for antipsychotic piperazinyldibenzothiazepine deriv., are prepd. by reaction of (substituted) 2-halonitrobenzenes with (substituted) thiosalicylic acids, redn. of the resulting II (R1-R8 = same as I; Y = NO2), and dehydrocondensation of II (Y = NH2). 2-Chloronitrobenzene was condensed with thiosalicylic acid in N,N-dimethylformamide using K2CO3 at 70.degree. for 6 h to give 98% II (R1-R8 = H, Y = NO2), which was reduced by H using Raney Ni and heated in refluxing PhMe to give I (R1-R8 = H).

IT **19806-43-0P 55114-91-5P**

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of dibenzothiazepines from halonitrobenzenes and thiosalicylic acids)

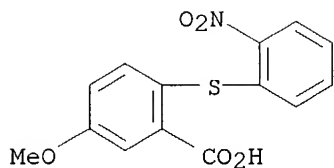
RN 19806-43-0 CAPLUS

CN Benzoic acid, 2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)

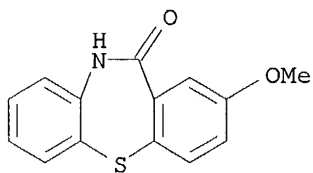


RN 55114-91-5 CAPLUS

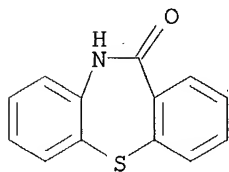
CN Benzoic acid, 5-methoxy-2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



IT 3158-77-8P 3159-07-7P, Dibenzo[b,f][1,4]thiazepin-
 11(10H)-one
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
 (Preparation)
 (prepn. of dibenzothiazepines from halonitrobenzenes and thiosalicylic
 acids)
 RN 3158-77-8 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methoxy- (7CI, 8CI, 9CI) (CA
 INDEX NAME)



RN 3159-07-7 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one (6CI, 7CI, 8CI, 9CI) (CA INDEX
 NAME)



L13 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1994:435589 CAPLUS

DOCUMENT NUMBER: 121:35589

TITLE: Novel reactions of spiro-sulfurane precursor sulfides and sulfoxides

AUTHOR(S): Kuti, M.; Rabai, J.; Kapovits, I.

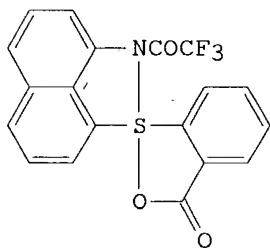
CORPORATE SOURCE: Dep. Org. Chem., L. Eotvos Univ., Budapest, H-1518, Hung.

SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1993), 85(1-4), 119-27
CODEN: PSSLEC; ISSN: 1042-6507

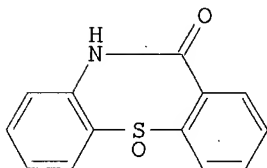
DOCUMENT TYPE: Journal

LANGUAGE: English

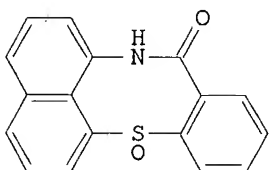
GI



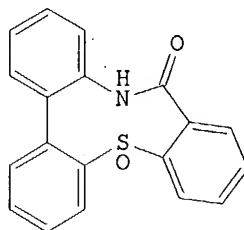
I



II



III



IV

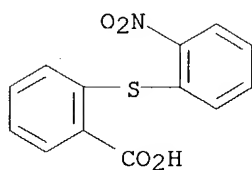
AB The SIV[C,C,N,O] spiro-sulfurane I and the lactam-sulfoxides II, III, and IV with seven-, eight- and nine-membered rings have been prepd. by oxidn. and dehydration of trifluoroacetylaminophenylcarboxyphenyl sulfides and sulfoxides, resp. A mechanism is proposed for the formation of lactam-sulfoxides. The prepn. of the starting sulfides and sulfoxides is also described.

IT 19806-43-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and redn. by iron)

RN 19806-43-0 CAPLUS

CN Benzoic acid, 2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



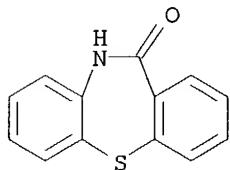
IT 3159-07-7P, Dibenzo[b,f][1,4]thiazepin-11(10H)-one

20290-48-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

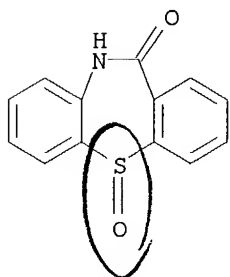
RN 3159-07-7 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

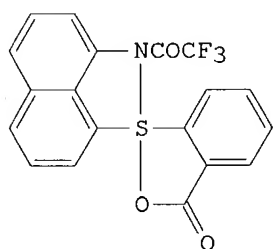


RN 20290-48-6 CAPLUS

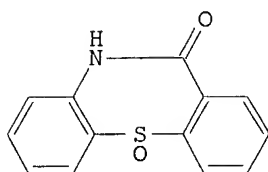
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 5-oxide (8CI, 9CI) (CA INDEX NAME)



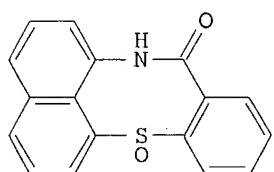
2943
 L21 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1994:435589 CAPLUS
 DOCUMENT NUMBER: 121:35589
 TITLE: Novel reactions of spiro-sulfurane precursor sulfides and sulfoxides
 AUTHOR(S): Kuti, M.; Rabai, J.; Kapovits, I.
 CORPORATE SOURCE: Dep. Org. Chem., L. Eotvos Univ., Budapest, H-1518, Hung.
 SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1993), 85(1-4), 119-27
 CODEN: PSSLEC; ISSN: 1042-6507
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



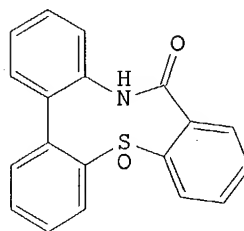
I



II



III



IV

AB The SIV[C,C,N,O] spiro-sulfurane I and the lactam-sulfoxides II, III, and IV with seven-, eight- and nine-membered rings have been prepared by oxidation and dehydration of trifluoroacetylaminophenylcarboxyphenyl sulfides and sulfoxides, resp. A mechanism is proposed for the formation of lactam-sulfoxides. The preparation of the starting sulfides and sulfoxides is also described.

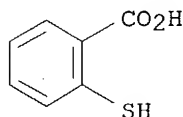
IT 147-93-3, Thiosalicylic acid

RL: RCT (Reactant); RACT (Reactant or reagent)

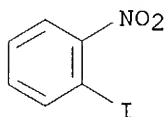
(coupling of, with iodonitrobenzene, iodonitrobiphenyl, and bromonaphthyltrifluoroacetamide)

RN 147-93-3 CAPLUS

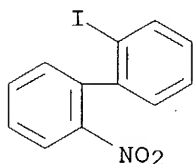
CN Benzoic acid, 2-mercapto- (9CI) (CA INDEX NAME)



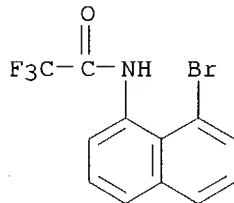
IT **609-73-4**, 1-Iodo-2-nitrobenzene **35882-95-2**,
 1,1'-Biphenyl, 2-iodo-2'-nitro- **155882-83-0**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (coupling of, with thiosalicylic acid)
 RN 609-73-4 CAPLUS
 CN Benzene, 1-iodo-2-nitro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



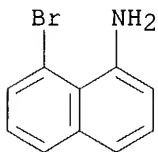
RN 35882-95-2 CAPLUS
 CN 1,1'-Biphenyl, 2-iodo-2'-nitro- (9CI) (CA INDEX NAME)



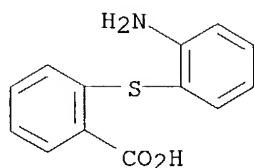
RN 155882-83-0 CAPLUS
 CN Acetamide, N-(8-bromo-1-naphthalenyl)-2,2,2-trifluoro- (9CI) (CA INDEX NAME)



IT **62456-34-2P**, 1-Naphthalenamine, 8-bromo- **114724-41-3P**
155586-27-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and acylation by trifluoroacetic anhydride)
 RN 62456-34-2 CAPLUS
 CN 1-Naphthalenamine, 8-bromo- (9CI) (CA INDEX NAME)

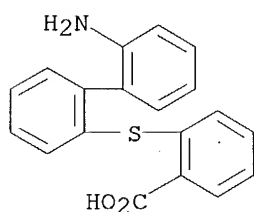


RN 114724-41-3 CAPLUS
 CN Benzoic acid, 2-[(2-aminophenyl)thio]-, hydrochloride (9CI) (CA INDEX NAME)



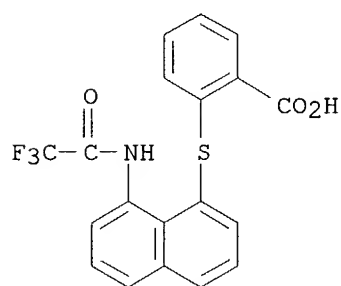
● HCl

RN 155586-27-9 CAPLUS
 CN Benzoic acid, 2-[(2'-amino[1,1'-biphenyl]-2-yl)thio]-, hydrochloride (9CI)
 (CA INDEX NAME)

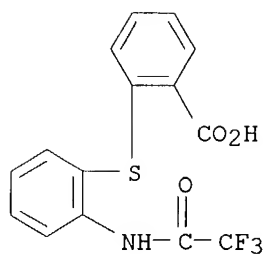


● HCl

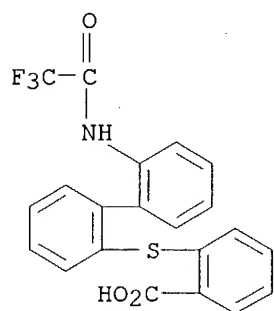
IT **155882-75-0P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and oxidation by phenyltrimethylammonium bromide)
 RN 155882-75-0 CAPLUS
 CN Benzoic acid, 2-[[8-[(trifluoroacetyl)amino]-1-naphthalenyl]thio]- (9CI)
 (CA INDEX NAME)



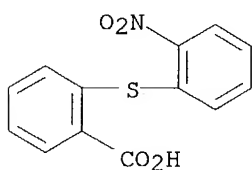
IT **155882-74-9P 155882-76-1P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and oxidation by tert-Bu hypochlorite)
 RN 155882-74-9 CAPLUS
 CN Benzoic acid, 2-[[2-[(trifluoroacetyl)amino]phenyl]thio]- (9CI) (CA INDEX NAME)



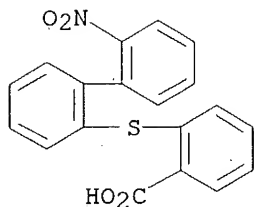
RN 155882-76-1 CAPLUS
 CN Benzoic acid, 2-[[2'-[(trifluoroacetyl)amino][1,1'-biphenyl]-2-yl]thio]-
 (9CI) (CA INDEX NAME)



IT **19806-43-0P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and reduction by iron)
 RN 19806-43-0 CAPLUS
 CN Benzoic acid, 2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



IT **155882-80-7P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and reduction with iron)
 RN 155882-80-7 CAPLUS
 CN Benzoic acid, 2-[(2'-nitro[1,1'-biphenyl]-2-yl)thio]- (9CI) (CA INDEX NAME)



IT 3159-07-7P, Dibenzo[b,f][1,4]thiazepin-11(10H)-one

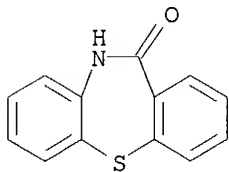
20290-48-6P 155586-25-7P 155882-81-8P

155882-82-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

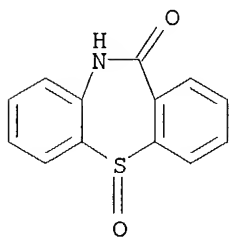
RN 3159-07-7 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



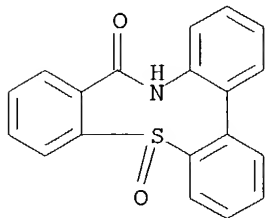
RN 20290-48-6 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 5-oxide (8CI, 9CI) (CA INDEX NAME)



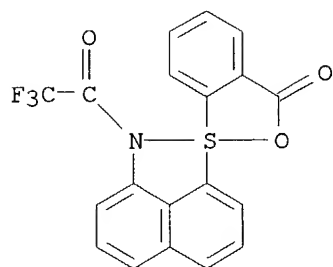
RN 155586-25-7 CAPLUS

CN Tribenzo[b,f,h][1,5]thiazonin-10(11H)-one, 5-oxide (9CI) (CA INDEX NAME)

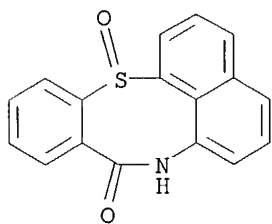


RN 155882-81-8 CAPLUS

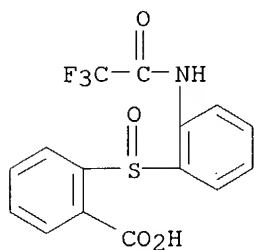
CN Spiro[3H-2,1-benzoxathiole-1,1'-λ4-[2H]naphth[1,8-cd]isothiazol]-3-one, 2'-(trifluoroacetyl)- (9CI) (CA INDEX NAME)



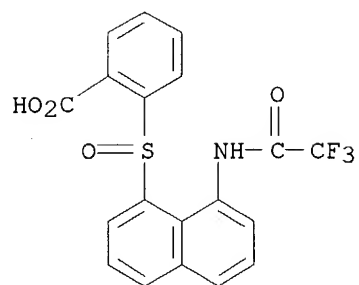
RN 155882-82-9 CAPLUS
 CN Benzo[g]naphtho[1,8-bc][1,5]thiazocin-8(7H)-one, 13-oxide (9CI) (CA INDEX NAME)



IT 155882-77-2P 155882-78-3P 155882-79-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as spiro-sulfurane precursor)
 RN 155882-77-2 CAPLUS
 CN Benzoic acid, 2-[[2-[(trifluoroacetyl)amino]phenyl]sulfinyl]- (9CI) (CA INDEX NAME)

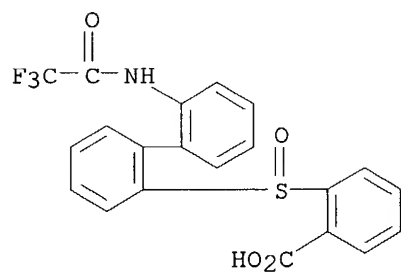


RN 155882-78-3 CAPLUS
 CN Benzoic acid, 2-[[8-[(trifluoroacetyl)amino]-1-naphthalenyl]sulfinyl]- (9CI) (CA INDEX NAME)

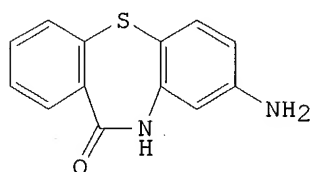


RN 155882-79-4 CAPLUS

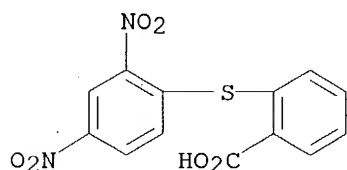
CN Benzoic acid, 2-[[2'-[(trifluoroacetyl)amino][1,1'-biphenyl]-2-yl]sulfinyl]- (9CI) (CA INDEX NAME)



L13 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1986:626505 CAPLUS
 DOCUMENT NUMBER: 105:226505
 TITLE: Synthesis and structural studies of
 8-amino-10,11-dihydro-5H-dibenzo[b,e][1,4]thiazepine-
 11-one
 AUTHOR(S): Joshi, B. C.; Pande, Jyoti
 CORPORATE SOURCE: Chem. Lab., Univ. Rajasthan, Jaipur, 302004, India
 SOURCE: Chemistry & Industry (London, United Kingdom) (1985),
 (24), 825-6
 CODEN: CHINAG; ISSN: 0009-3068
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 105:226505
 GI

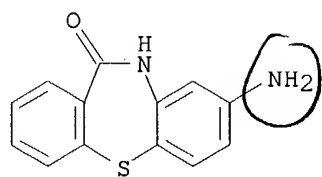


AB o-HO₂CC₆H₄SC₆H₃(O₂N)₂-2,4, prepd. from o-HSC₆H₄CO₂H and 2,4-(O₂N)₂C₆H₃Cl
 was reduced to o-HO₂CC₆H₄SC₆H₃(NH₂)₂-2,4, which was cyclized by H₃PO₄ to
 give the title compd. (I).
 IT **33840-90-3P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and redn. of)
 RN 33840-90-3 CAPLUS
 CN Benzoic acid, 2-[(2,4-dinitrophenyl)thio]- (9CI) (CA INDEX NAME)

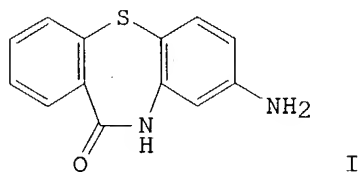


IT **105554-89-0P**
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and spectra of)
 RN 105554-89-0 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-amino- (9CI) (CA INDEX NAME)

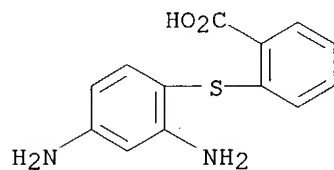
10/030,251



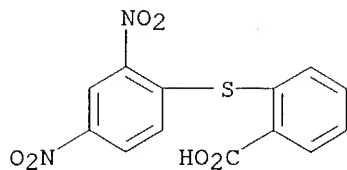
32/13
L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1986:626505 CAPLUS
DOCUMENT NUMBER: 105:226505
TITLE: Synthesis and structural studies of
8-amino-10,11-dihydro-5H-dibenzo[b,e][1,4]thiazepine-
11-one
AUTHOR(S): Joshi, B. C.; Pande, Jyoti
CORPORATE SOURCE: Chem. Lab., Univ. Rajasthan, Jaipur, 302004, India
SOURCE: Chemistry & Industry (London, United Kingdom) (1985),
(24), 825-6
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:226505
GI



AB o-HO2CC6H4SC6H3(O2N)2-2,4, prepared from o-HSC6H4CO2H and 2,4-(O2N)2C6H3Cl
was reduced to o-HO2CC6H4SC6H3(NH2)2-2,4, which was cyclized by H3PO4 to
give the title compound(I).
IT 105554-88-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and intramol. cyclization of, dibenzothiazepinone derivative
from)
RN 105554-88-9 CAPLUS
CN Benzoic acid, 2-[(2,4-diaminophenyl)thio]- (9CI) (CA INDEX NAME)



IT 33840-90-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reduction of)
RN 33840-90-3 CAPLUS
CN Benzoic acid, 2-[(2,4-dinitrophenyl)thio]- (9CI) (CA INDEX NAME)

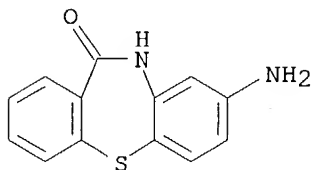


IT 105554-89-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectra of)

RN 105554-89-0 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-amino- (9CI) (CA INDEX NAME)

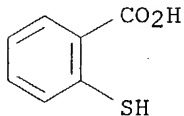


IT 147-93-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chlorodinitrobenzene)

RN 147-93-3 CAPLUS

CN Benzoic acid, 2-mercapto- (9CI) (CA INDEX NAME)

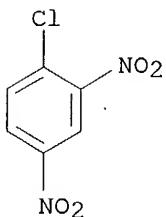


IT 97-00-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with mercaptoacetic acid)

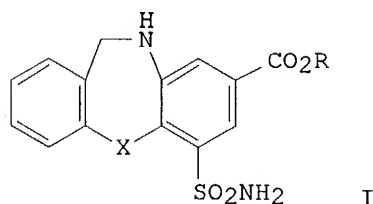
RN 97-00-7 CAPLUS

CN Benzene, 1-chloro-2,4-dinitro- (8CI, 9CI) (CA INDEX NAME)



10/030,251

L13 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1978:499969 CAPLUS
DOCUMENT NUMBER: 89:99969
TITLE: 8-Carboxy-6-sulfamoyldibenz[b,f][1,4]oxazepines and
-thiazepines as potential high-ceiling diuretics
AUTHOR(S): Allen, Richard C.; Reitano, Philip A.; Urbach, .
Hansjoerg
CORPORATE SOURCE: Chem. Res. Dep., Hoechst-Roussel Pharm. Inc.,
Somerville, NJ, USA
SOURCE: Journal of Medicinal Chemistry (1978), 21(8), 838-40
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

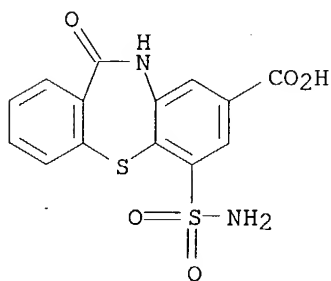


AB Five title compds. I (X = O or S, Y = O or H₂, R = H or Me), conformationally rigid analogs of furosemide [54-31-9], were synthesized and tested for diuretic activity. Only I; (X = Y = O, R = Me) [66984-09-6] and I; (X = O, Y = H₂, R = H) [66984-10-9] had natriuretic activity in rats and none of the compds. increased urinary vol. Apparently, conformational mobility of the 4-substituent of 3-amino-5-sulfamoylbenzoates is required for diuretic activity.

IT **66983-99-1P 66984-00-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. and diuretic activity of)

RN 66983-99-1 CAPLUS

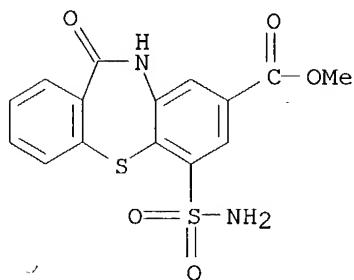
CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro-11-oxo- (9CI) (CA INDEX NAME)



RN 66984-00-7 CAPLUS

10/030,251

CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro-11-oxo-, methyl ester (9CI) (CA INDEX NAME)

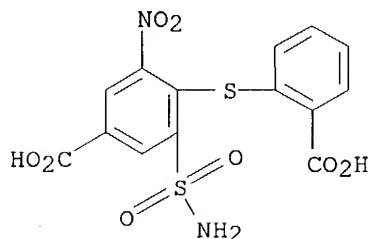


IT 66983-97-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and redn. of)

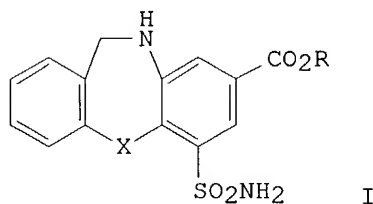
RN 66983-97-9 CAPLUS

CN Benzoic acid, 3-(aminosulfonyl)-4-[(2-carboxyphenyl)thio]-5-nitro- (9CI) (CA INDEX NAME)



4913

L15 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1978:499969 CAPLUS
 DOCUMENT NUMBER: 89:99969
 TITLE: 8-Carboxy-6-sulfamyl-dibenz[b,f][1,4]oxazepines and
 -thiazepines as potential high-ceiling diuretics
 AUTHOR(S): Allen, Richard C.; Reitano, Philip A.; Urbach,
 Hansjoerg
 CORPORATE SOURCE: Chem. Res. Dep., Hoechst-Roussel Pharm. Inc.,
 Somerville, NJ, USA
 SOURCE: Journal of Medicinal Chemistry (1978), 21(8), 838-40
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 89:99969
 GI



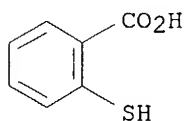
AB Five title compds. I (X = O or S, Y = O or H₂, R = H or Me), conformationally rigid analogs of furosemide [54-31-9], were synthesized and tested for diuretic activity. Only I; (X = Y = O, R = Me) [66984-09-6] and I; (X = O, Y = H₂, R = H) [66984-10-9] had natriuretic activity in rats and none of the compds. increased urinary volume. Apparently, conformational mobility of the 4-substituent of 3-amino-5-sulfamylbenzoates is required for diuretic activity.

IT 147-93-3

RL: BIOL (Biological study)
 (condensation of, with chloronitrosulfamylbenzoate)

RN 147-93-3 CAPLUS

CN Benzoic acid, 2-mercapto- (9CI) (CA INDEX NAME)

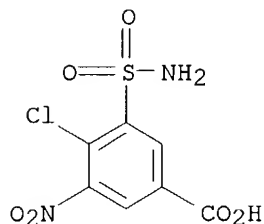


IT 22892-96-2

RL: BIOL (Biological study)
 (condensation of, with thiosalicylate)

RN 22892-96-2 CAPLUS

CN Benzoic acid, 3-(aminosulfonyl)-4-chloro-5-nitro- (9CI) (CA INDEX NAME)

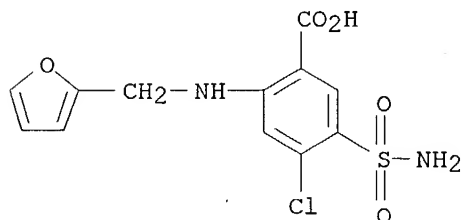


IT 54-31-9DP, analog 66983-99-1P 66984-00-7P
 66984-01-8P 66984-07-4DP, derivs. 66984-08-5DP
 , derivs. 66984-09-6P 66984-10-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation and diuretic activity of)

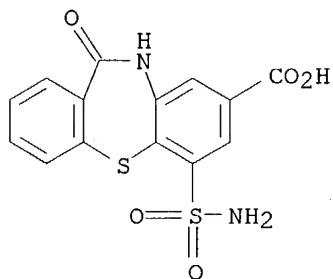
RN 54-31-9 CAPLUS

CN Benzoic acid, 5-(aminosulfonyl)-4-chloro-2-[(2-furanylmethyl)amino]- (9CI)
 (CA INDEX NAME)



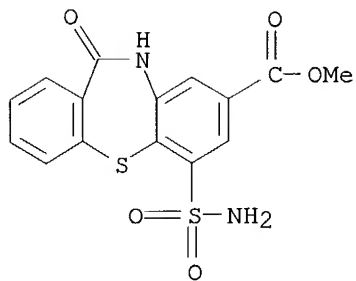
RN 66983-99-1 CAPLUS

CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro-11-oxo- (9CI) (CA INDEX NAME)



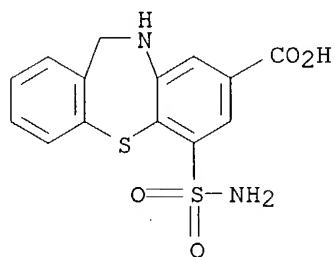
RN 66984-00-7 CAPLUS

CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro-11-oxo-, methyl ester (9CI) (CA INDEX NAME)



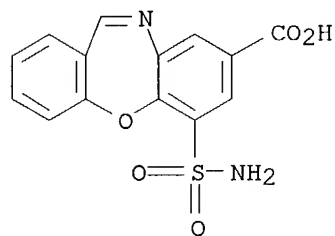
RN 66984-01-8 CAPLUS

CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro- (9CI) (CA INDEX NAME)



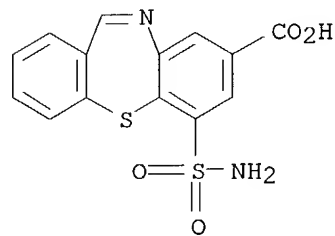
RN 66984-07-4 CAPLUS

CN Dibenzo[b,f][1,4]oxazepine-8-carboxylic acid, 6-(aminosulfonyl)- (9CI) (CA INDEX NAME)



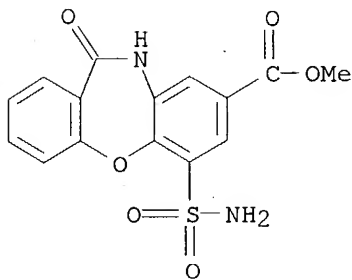
RN 66984-08-5 CAPLUS

CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)- (9CI) (CA INDEX NAME)



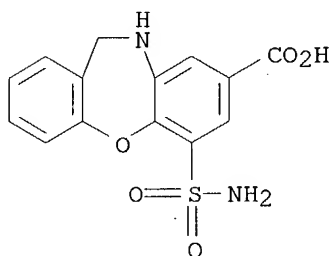
RN 66984-09-6 CAPLUS

CN Dibenzo[b,f][1,4]oxazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro-11-oxo-, methyl ester (9CI) (CA INDEX NAME)



RN 66984-10-9 CAPLUS

CN Dibenzo[b,f][1,4]oxazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro- (9CI) (CA INDEX NAME)

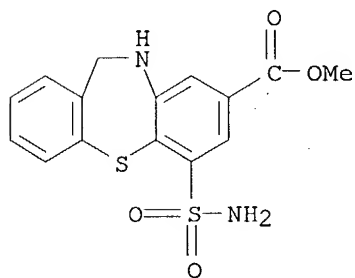


IT 66984-03-0P 66984-05-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrolysis of)

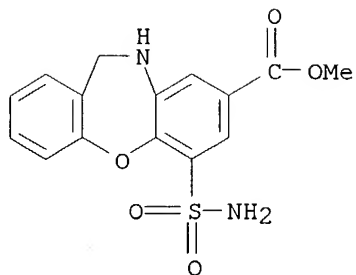
RN 66984-03-0 CAPLUS

CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro-, methyl ester (9CI) (CA INDEX NAME)



RN 66984-05-2 CAPLUS

CN Dibenzo[b,f][1,4]oxazepine-8-carboxylic acid, 6-(aminosulfonyl)-10,11-dihydro-, methyl ester (9CI) (CA INDEX NAME)



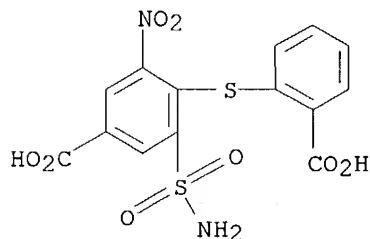
IT 66983-97-9P 66984-02-9P 66984-04-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reduction of)

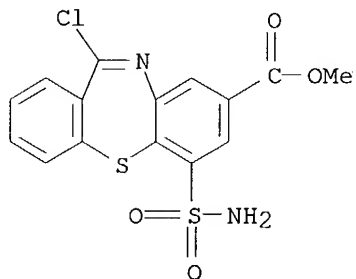
RN 66983-97-9 CAPLUS

CN Benzoic acid, 3-(aminosulfonyl)-4-[(2-carboxyphenyl)thio]-5-nitro- (9CI)
(CA INDEX NAME)



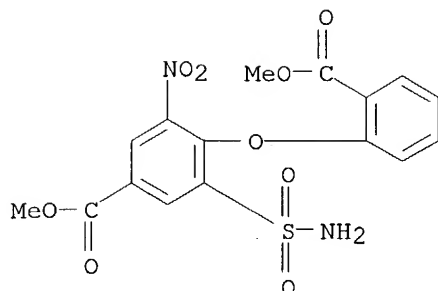
RN 66984-02-9 CAPLUS

CN Dibenzo[b,f][1,4]thiazepine-8-carboxylic acid, 6-(aminosulfonyl)-11-chloro-, methyl ester (9CI) (CA INDEX NAME)



RN 66984-04-1 CAPLUS

CN Benzoic acid, 3-(aminosulfonyl)-4-[2-(methoxycarbonyl)phenoxy]-5-nitro-, methyl ester (9CI) (CA INDEX NAME)



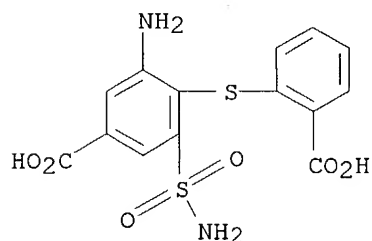
IT 66983-98-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and thermal cyclodehydration of)

RN 66983-98-0 CAPLUS

CN Benzoic acid, 3-amino-5-(aminosulfonyl)-4-[(2-carboxyphenyl)thio]- (9CI)
(CA INDEX NAME)

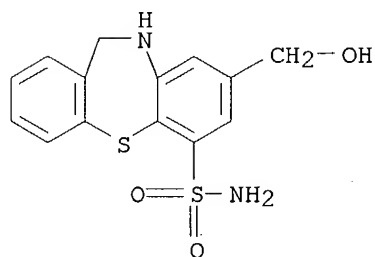


IT 66984-06-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 66984-06-3 CAPLUS

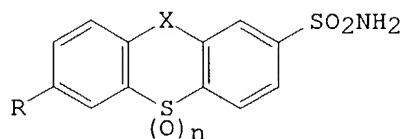
CN Dibenzo[b,f][1,4]thiazepine-6-sulfonamide, 10,11-dihydro-8-(hydroxymethyl)-
(9CI) (CA INDEX NAME)



10/030,251

13 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1978:22940 CAPLUS
DOCUMENT NUMBER: 88:22940
TITLE: Tricyclic sulfonamides
INVENTOR(S): Cross, Peter Edward; Dickinson, Roger Peter
PATENT ASSIGNEE(S): Pfizer Ltd., UK
SOURCE: Brit., 13 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1480553	A	19770720	GB 1975-25129	19760603
PRIORITY APPLN. INFO.: GI			GB 1975-25129	19760603



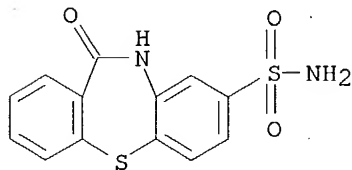
AB Seventeen title compds. I (R = H, Cl, CF₃; X = bond, CH₂, NAc, NH, CONH, NHCO, CO, NH; n = 0, 2), useful as cerebral vasodilators (no data), were prepd. by std. methods. E.g., thioxanthene-2-sulfonyl chloride with excess NH₃ gave I (R = H, X = CH₂, n = 0) which on H₂O₂ oxidn. in AcOH gave I (R = H, X = CH₂, n = 2). I (R = Cl, X = NAc, n = 0) was prepd. from [2,4-(H₂N)(H₂NSO₂)C₆H₃]₂S by sequential treatment with 2,5-Cl₂C₆H₃NO₂, acetylation, and refluxing with alc. KOH in Me₂CO. Many I show anticonvulsant activity (no data).

IT 65192-76-9P 65192-80-5P 65192-85-0P
65192-86-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(cerebral vasodilator, prepn. of)

RN 65192-76-9 CAPLUS

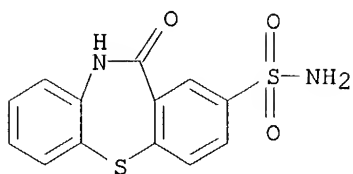
CN Dibenzo[b,f][1,4]thiazepine-8-sulfonamide, 10,11-dihydro-11-oxo- (9CI)
(CA INDEX NAME)



RN 65192-80-5 CAPLUS

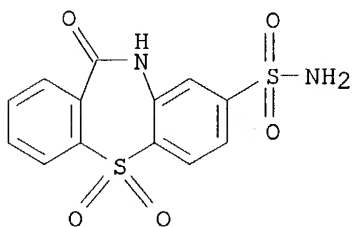
CN Dibenzo[b,f][1,4]thiazepine-2-sulfonamide, 10,11-dihydro-11-oxo- (9CI)
(CA INDEX NAME)

10/030,251



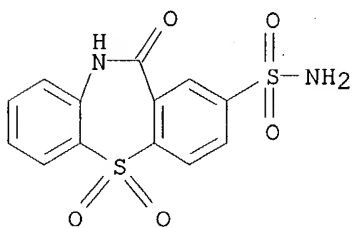
RN 65192-85-0 CAPLUS

CN Dibenzo[b,f][1,4]thiazepine-8-sulfonamide, 10,11-dihydro-11-oxo-, 5,5-dioxide (9CI) (CA INDEX NAME)



RN 65192-86-1 CAPLUS

CN Dibenzo[b,f][1,4]thiazepine-2-sulfonamide, 10,11-dihydro-11-oxo-, 5,5-dioxide (9CI) (CA INDEX NAME)

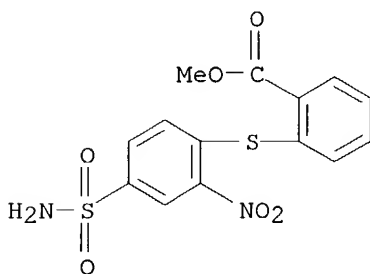


IT 65192-74-7P 65192-78-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and redn. of)

RN 65192-74-7 CAPLUS

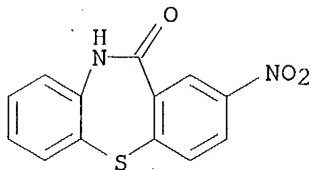
CN Benzoic acid, 2-[[4-(aminosulfonyl)-2-nitrophenyl]thio]-, methyl ester (9CI) (CA INDEX NAME)



10/030,251

RN 65192-78-1 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-nitro- (9CI) (CA INDEX NAME)

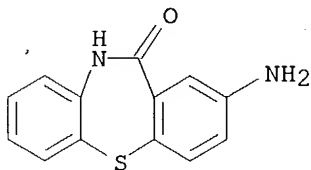


IT 65192-79-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and sulfamoylation of)

RN 65192-79-2 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-amino- (9CI) (CA INDEX NAME)



~~L13~~ ANSWER 6 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1976:105557 CAPLUS

DOCUMENT NUMBER: 84:105557

TITLE: A novel synthesis of dibenzo[b,f][1,4]thiazepin-11(10H)one 5,5-dioxides

AUTHOR(S): Bennett, O. Francis; Johnson, James; Galletto, Sandra

CORPORATE SOURCE: Dep. Chem., Boston Coll., Chestnut Hill, MA, USA

SOURCE: Journal of Heterocyclic Chemistry (1975), 12(6), 1211-13

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

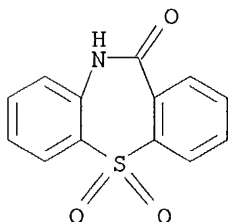
AB Treatment of thioxanthen-9-one 10,10-dioxides I (R = H, Me, MeO) with NaNH₂ in liq. NH₃ gave dibenzo[b,f][1,4]thiazepin-11(10H)one 5,5-dioxides II (R = H, Me, R1 = H; R = H, R1 = MeO; resp.) II (R = Me, R1 = H) was prepd. from Me 5-methylthiosalicylate.

IT **22871-33-6P 58755-60-5P 58755-62-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and methylation of)

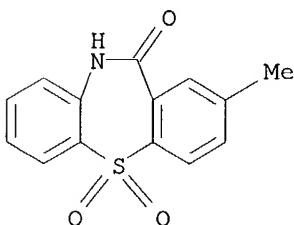
RN 22871-33-6 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 5,5-dioxide (6CI, 8CI, 9CI) (CA INDEX NAME)



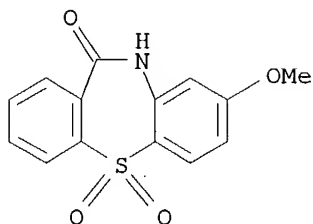
RN 58755-60-5 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methyl-, 5,5-dioxide (9CI) (CA INDEX NAME)



RN 58755-62-7 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methoxy-, 5,5-dioxide (9CI) (CA INDEX NAME)

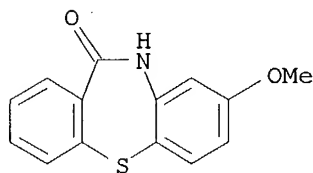


IT 3159-05-5P 58755-60-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and oxidn. of)

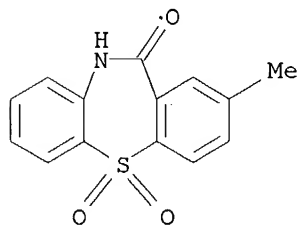
RN 3159-05-5 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 58755-60-5 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methyl-, 5,5-dioxide (9CI) (CA INDEX NAME)

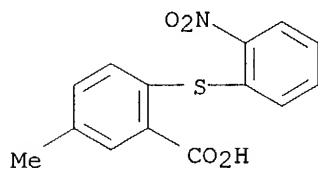


IT 58755-65-0P 58755-67-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and redn. of)

RN 58755-65-0 CAPLUS

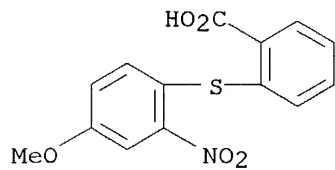
CN Benzoic acid, 5-methyl-2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



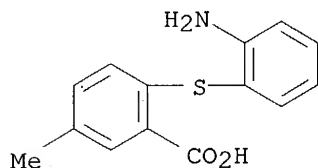
10/030,251

RN 58755-67-2 CAPLUS

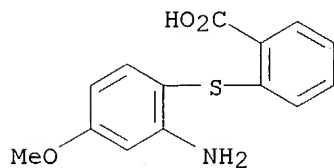
CN Benzoic acid, 2-[(4-methoxy-2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



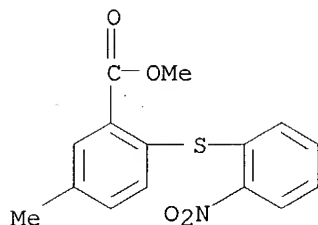
6813
L12 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1976:105557 CAPLUS
DOCUMENT NUMBER: 84:105557
TITLE: A novel synthesis of dibenzo[b,f][1,4]thiazepin-11(10H)one 5,5-dioxides
AUTHOR(S): Bennett, O. Francis; Johnson, James; Galletto, Sandra
CORPORATE SOURCE: Dep. Chem., Boston Coll., Chestnut Hill, MA, USA
SOURCE: Journal of Heterocyclic Chemistry (1975), 12(6), 1211-13
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 84:105557
GI For diagram(s), see printed CA Issue.
AB Treatment of thioxanthen-9-one 10,10-dioxides I (R = H, Me, MeO) with NaNH2 in liquid NH3 gave dibenzo[b,f][1,4]thiazepin-11(10H)one 5,5-dioxides II (R = H, Me, R1 = H; R = H, R1 = MeO; resp.) II (R = Me, R1 = H) was prepared from Me 5-methylthiosalicylate.
IT 58755-66-1P 58755-68-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 58755-66-1 CAPLUS
CN Benzoic acid, 2-[(2-aminophenyl)thio]-5-methyl- (9CI) (CA INDEX NAME)



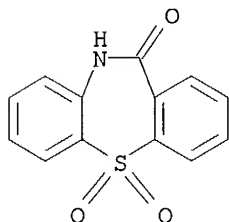
RN 58755-68-3 CAPLUS
CN Benzoic acid, 2-[(2-amino-4-methoxyphenyl)thio]- (9CI) (CA INDEX NAME)



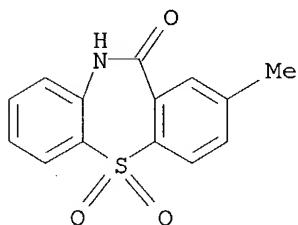
IT 58755-64-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 58755-64-9 CAPLUS
CN Benzoic acid, 5-methyl-2-[(2-nitrophenyl)thio]-, methyl ester (9CI) (CA INDEX NAME)



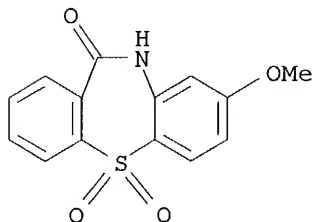
IT 22871-33-6P 58755-60-5P 58755-62-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and methylation of)
 RN 22871-33-6 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 5,5-dioxide (6CI, 8CI, 9CI) (CA
 INDEX NAME)



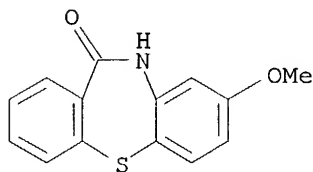
RN 58755-60-5 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methyl-, 5,5-dioxide (9CI) (CA
 INDEX NAME)



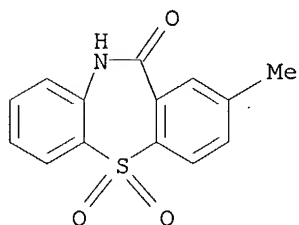
RN 58755-62-7 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methoxy-, 5,5-dioxide (9CI) (CA
 INDEX NAME)



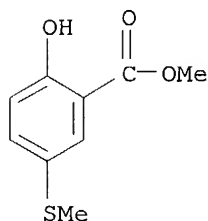
IT **3159-05-5P 58755-60-5P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and oxidation of)
 RN 3159-05-5 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methoxy- (6CI, 7CI, 8CI, 9CI)
 (CA INDEX NAME)



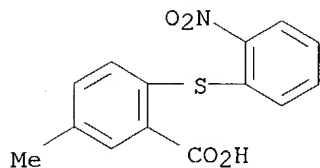
RN 58755-60-5 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methyl-, 5,5-dioxide (9CI) (CA
 INDEX NAME)



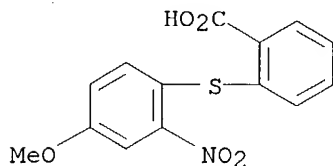
IT **59699-19-3P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reaction with iodonitrobenzene)
 RN 59699-19-3 CAPLUS
 CN Benzoic acid, 2-hydroxy-5-(methylthio)-, methyl ester (9CI) (CA INDEX
 NAME)



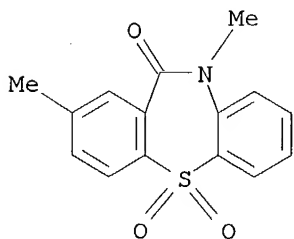
IT **58755-65-0P 58755-67-2P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reduction of)
 RN 58755-65-0 CAPLUS
 CN Benzoic acid, 5-methyl-2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



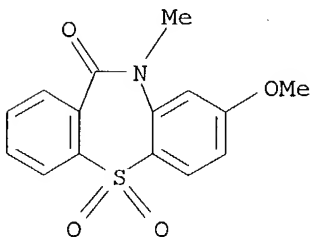
RN 58755-67-2 CAPLUS
 CN Benzoic acid, 2-[(4-methoxy-2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



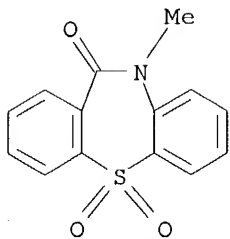
IT **58755-61-6P 58755-63-8P 58790-38-8P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 58755-61-6 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2,10-dimethyl-, 5,5-dioxide (9CI)
 (CA INDEX NAME)



RN 58755-63-8 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methoxy-10-methyl-, 5,5-dioxide
 (9CI) (CA INDEX NAME)



RN 58790-38-8 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 10-methyl-, 5,5-dioxide (9CI) (CA INDEX NAME)

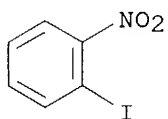


IT 609-73-4 58755-70-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methyl methylthiosalicylate)

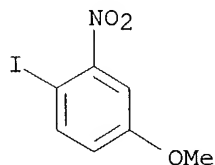
RN 609-73-4 CAPLUS

CN Benzene, 1-iodo-2-nitro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 58755-70-7 CAPLUS

CN Benzene, 1-iodo-4-methoxy-2-nitro- (9CI) (CA INDEX NAME)

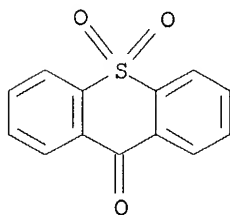


IT 3166-15-2 14753-21-0 58755-69-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sodium amide, dibenzothiazepinone dioxide from)

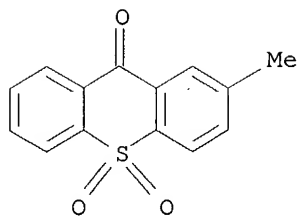
RN 3166-15-2 CAPLUS

CN 9H-Thioxanthen-9-one, 10,10-dioxide (9CI) (CA INDEX NAME)



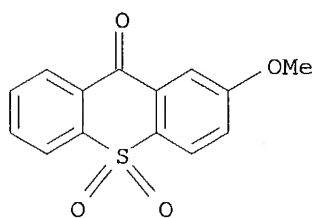
RN 14753-21-0 CAPLUS

CN 9H-Thioxanthen-9-one, 2-methyl-, 10,10-dioxide (9CI) (CA INDEX NAME)



RN 58755-69-4 CAPLUS

CN 9H-Thioxanthene-9-one, 2-methoxy-, 10,10-dioxide (9CI) (CA INDEX NAME)



L13 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1975:140094 CAPLUS

DOCUMENT NUMBER: 82:140094

TITLE: Synthesis of 2-methoxydibenzo[b,f][1,4]-thiazepin-11(10H)-one 5,5-dioxide

AUTHOR(S): Bennett, O. Francis; Johnson, James; Tramondozzi, John

CORPORATE SOURCE: Dep. Chem., Boston Coll., Chestnut Hill, MA, USA

SOURCE: Organic Preparations and Procedures International (1974), 6(6), 287-93

CODEN: OPPIAK; ISSN: 0030-4948

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

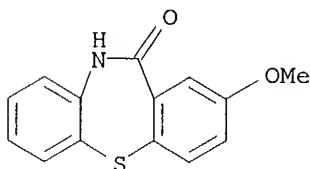
AB The title compd. (I, n = 2) was prepd. from the nitrobenzoate II (R = Me, R1 = NO2) in 8 steps. Thus II (R = Me, R1 = NO2) was reduced to II (R = Me, R1 = NH2), hydrolyzed to II (R = H, R1 = NH2), deaminated and treated with Na2S to give II (R = H, R1 = SH), which was esterified and treated with 2-O2NC6H4I and hydrolyzed to give II (R = H, R1 = 2-O2NC6H4S). FeSO4-NH4OH redn. gave II (R = H, R1 = 2-H2NC6H4S), which was cyclized to I (n = 0) and oxidized to I (n = 2).

IT 3158-77-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of)

RN 3158-77-8 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methoxy- (7CI, 8CI, 9CI) (CA INDEX NAME)

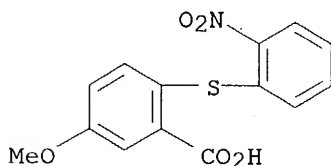


IT 55114-91-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)

RN 55114-91-5 CAPLUS

CN Benzoic acid, 5-methoxy-2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



IT 55114-93-7P

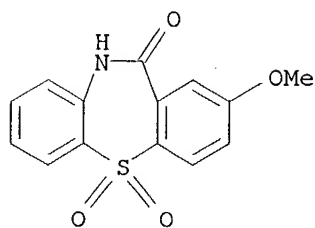
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 55114-93-7 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methoxy-, 5,5-dioxide (9CI) (CA

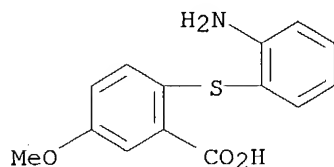
10/030,251

INDEX NAME)

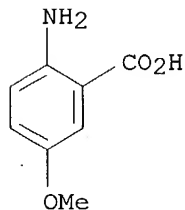


7/8/13

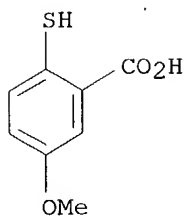
L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1975:140094 CAPLUS
 DOCUMENT NUMBER: **82:140094**
 TITLE: Synthesis of 2-methoxydibenzo[b,f](1,4)-thiazepin-11(10H)-one 5,5-dioxide
 AUTHOR(S): Bennett, O. Francis; Johnson, James; Tramondozzi, John
 CORPORATE SOURCE: Dep. Chem., Boston Coll., Chestnut Hill, MA, USA
 SOURCE: Organic Preparations and Procedures International (1974), 6(6), 287-93
 CODEN: OPPIAK; ISSN: 0030-4948
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB The title compound (I, n = 2) was prepared from the nitrobenzoate II (R = Me, R1 = NO2) in 8 steps. Thus II (R = Me, R1 = NO2) was reduced to II (R = Me, R1 = NH2), hydrolyzed to II (R = H, R1 = NH2), deaminated and treated with Na2S to give II (R = H, R1 = SH), which was esterified and treated with 2-O2NC6H4I and hydrolyzed to give II (R = H, R1 = 2-O2NC6H4S). FeSO4-NH4OH reduction gave II (R = H, R1 = 2-H2NC6H4S), which was cyclized to I (n = 0) and oxidized to I (n = 2).
 IT **55114-92-6P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and cyclization of)
 RN 55114-92-6 CAPLUS
 CN Benzoic acid, 2-[(2-aminophenyl)thio]-5-methoxy- (9CI) (CA INDEX NAME)



IT **6705-03-9P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and deamination of)
 RN 6705-03-9 CAPLUS
 CN Benzoic acid, 2-amino-5-methoxy- (9CI) (CA INDEX NAME)



IT **16807-37-7P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and esterification of)
 RN 16807-37-7 CAPLUS
 CN Benzoic acid, 2-mercapto-5-methoxy- (9CI) (CA INDEX NAME)



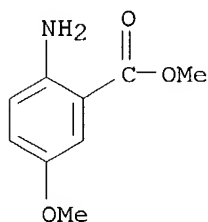
IT **2475-80-1P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

RN 2475-80-1 CAPLUS

CN Benzoic acid, 2-amino-5-methoxy-, methyl ester (9CI) (CA INDEX NAME)



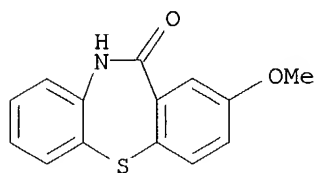
IT **3158-77-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidation of)

RN 3158-77-8 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methoxy- (7CI, 8CI, 9CI) (CA INDEX NAME)



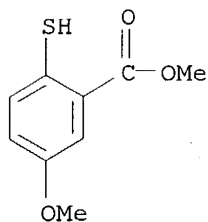
IT **55114-90-4P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with nitro(iodo)benzene)

RN 55114-90-4 CAPLUS

CN Benzoic acid, 2-mercapto-5-methoxy-, methyl ester (9CI) (CA INDEX NAME)

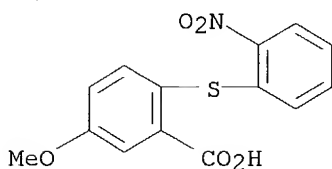


IT 55114-91-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 55114-91-5 CAPLUS

CN Benzoic acid, 5-methoxy-2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)

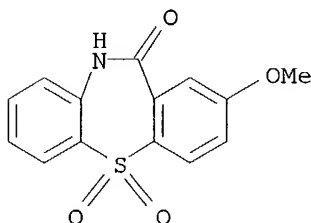


IT 55114-93-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 55114-93-7 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-methoxy-, 5,5-dioxide (9CI) (CA INDEX NAME)

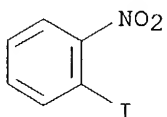


IT 609-73-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methoxythiosalicylate)

RN 609-73-4 CAPLUS

CN Benzene, 1-iodo-2-nitro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



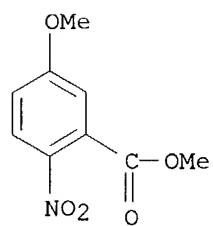
IT 2327-45-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(reduction of)

RN 2327-45-9 CAPLUS

CN Benzoic acid, 5-methoxy-2-nitro-, methyl ester (9CI) (CA INDEX NAME)



10/030,251

~~113~~ ANSWER 8 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1974:3563 CAPLUS

DOCUMENT NUMBER: 80:3563

TITLE: Dibenzo[b,f][1,4]thiazepine derivatives

INVENTOR(S): Schmutz, Jean; Hunziker, Fritz; Kuenzle, Franz M.

PATENT ASSIGNEE(S): Wander, Dr. A., A.-G.

SOURCE: Fr. Demande, 27 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2162575	A1	19730720	FR 1972-43707	19721208
FR 2162575	B1	19760702		
CH 560213	A	19750327	CH 1971-17925	19711209
BE 792426	A1	19730607	BE 1972-125052	19721207
JP 48064090	A2	19730905	JP 1972-122128	19721207
GB 1411587	A	19751029	GB 1972-56659	19721208
			CH 1971-17925	19711209

PRIORITY APPLN. INFO.:

GI For diagram(s), see printed CA Issue.

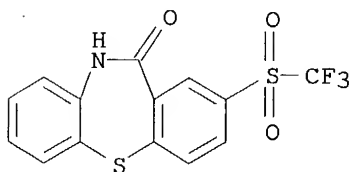
AB Piperazinyl-benzothiazepines I (R = H, Me, CH₂CH₂OH, (CH₂)₃OH, CH₂CHMeOH, Et, CH₂CH₂OMe, CH₂CH₂OAc) were prepd. for use as sedatives, tranquilizers, antidepressants, and antiemetics. Thus, 2,5-Br(MeS)C₆H₃CO₂H was chlorinated, then fluorinated, and oxidized to 2,5-Br(F₃CSO₂)C₆H₃CO₂H, which was treated with 2-H₂NC₆H₄SH and cyclized to 2-trifluoromethylsulfonyl-10,11-dihydro-11-oxodibenzo[b,f][1,4]thiazepine. Treatment with 4-methylpiperazine gave I (R = Me).

IT **42252-15-3P 42252-27-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 42252-15-3 CAPLUS

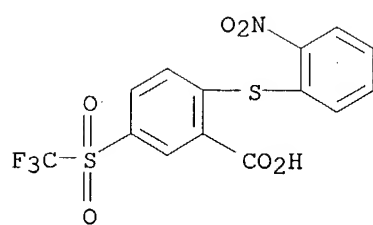
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-[(trifluoromethyl)sulfonyl]-
(9CI) (CA INDEX NAME)



RN 42252-27-7 CAPLUS

CN Benzoic acid, 2-[(2-nitrophenyl)thio]-5-[(trifluoromethyl)sulfonyl]- (9CI)
(CA INDEX NAME)

10/030,251



see
8913

L13 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1973:453389 CAPLUS
 DOCUMENT NUMBER: 79:53389
 TITLE: 11-Piperazinyl-2-[(trifluoromethyl)sulfonyl]
 dibenzo[b,f][1,4]-thiazepines
 INVENTOR(S): Schmutz, Jean; Hunziker, Fritz; Kuenzle, Franz M.
 PATENT ASSIGNEE(S): Wander A.-G.
 SOURCE: Ger. Offen., 30 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2259568	A1	19730614	DE 1972-2259568	19721206
CH 560213	A	19750327	CH 1971-17925	19711209
BE 792426	A1	19730607	BE 1972-125052	19721207
JP 48064090	A2	19730905	JP 1972-122128	19721207
GB 1411587	A	19751029	GB 1972-56659	19721208
			CH 1971-17925	19711209

PRIORITY APPLN. INFO.:

GI For diagram(s), see printed CA Issue.

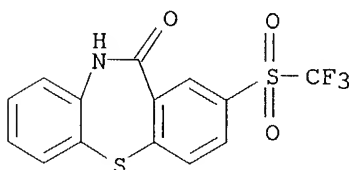
AB Eight title compds. [I, R = H, Me, Et, CH₂CH₂OH, (CH₂)₃OH, CH₂CH₂OMe, CH₂CH₂OAc, or CH₂CHMeOH] were prepd. by reaction of II or III with piperazines, by cyclization of 2-H₂NC₆-H₄SC₆H₃(SO₂CF₃)COA-4,2 (A = piperazinyl residues), and optionally by substitution of I (R = H). I were useful as sedatives, neuroleptics, neurotropic antidepressants, and anti-emetics.

IT **42252-15-3P 42252-27-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 42252-15-3 CAPLUS

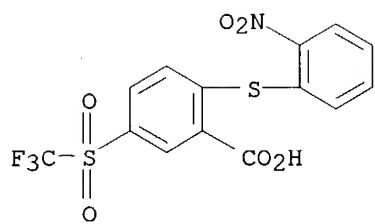
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 2-[(trifluoromethyl)sulfonyl]-
 (9CI) (CA INDEX NAME)



RN 42252-27-7 CAPLUS

CN Benzoic acid, 2-[(2-nitrophenyl)thio]-5-[(trifluoromethyl)sulfonyl]- (9CI)
 (CA INDEX NAME)

10/030,251



133 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1966:490113 CAPLUS

DOCUMENT NUMBER: 65:90113

ORIGINAL REFERENCE NO.: 65:16829f-g

TITLE: Nuclear magnetic resonance of benzobisheterocyclic compounds

AUTHOR(S): Grandolini, Giuliano; Ricci, Adolfo; Martani, Alfio; Monache, France Delle

CORPORATE SOURCE: Univ. Perugia, Italy

SOURCE: Journal of Heterocyclic Chemistry (1966), 3(3), 302-10

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

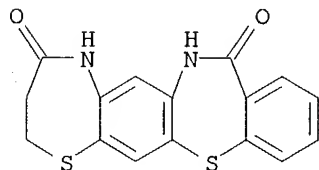
LANGUAGE: English

AB The N.M.R. spectra of 49 benzobisheterocyclic compds. containing various heterocycles were detd. The observed spectral data made possible the elucidation of the structure and also clarified the influences of the heterocyclic substituents and of heterocyclic rings on chem. shift values of the aromatic protons. 25 references.

IT 13399-10-5, 1,5-Benzothiazepino[8,7-b][1,4]benzothiazepine-4,8(5H,7H)-dione, 2,3-dihydro- (nuclear magnetic resonance of)

RN 13399-10-5 CAPLUS

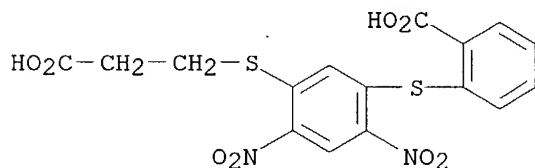
CN 1,5-Benzothiazepino[8,7-b][1,4]benzothiazepine-4,8(5H,7H)-dione, 2,3-dihydro- (7CI, 8CI) (CA INDEX NAME)



IT 13399-40-1, Benzoic acid, o-[[5-[(2-carboxyethyl)thio]-2,4-dinitrophenyl]thio]- (prepn. of)

RN 13399-40-1 CAPLUS

CN Benzoic acid, o-[[5-[(2-carboxyethyl)thio]-2,4-dinitrophenyl]thio]- (7CI, 8CI) (CA INDEX NAME)



~~113~~ ANSWER 11 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1961:137637 CAPLUS
 DOCUMENT NUMBER: 55:137637
 ORIGINAL REFERENCE NO.: 55:26001b-i
 TITLE: Basically substituted heterocyclic compounds
 INVENTOR(S): Hoffmann, Karl; Urech, Ernst
 PATENT ASSIGNEE(S): C I B A Ltd.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1062246		19590730	DE	
GB 869089			GB	

GI For diagram(s), see printed CA Issue.

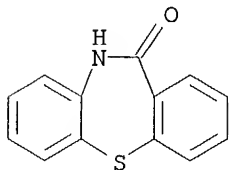
AB 10-(Tertiary-aminoalkyl)-11-oxo-dibenzo[b,f]-1-thia-4-aza-2,6-cycloheptadienes effective as antihistamines and for the treatment of asthma, were made by treating substituted o-nitrochlorobenzenes with an alk. soln. of Me thiosalicylate (I) to prep. Me 2'-nitrodiphenyl sulfide-2'-carboxylate, which gave on redn. the amino analog, which gave by heating the heterocyclic compd., which was treated with reactive aminoalkyl alcs. or esters in the presence of condensing agents, such as alk. metals, their amides or hydrides. Thus, 112 g. I was refluxed in 300 cc. anhyd. MeOH with 17 g. Na 10 min. and then treated with 130 g. 3-nitro-4-chlorotoluene. After refluxing 2.5 hrs., the hot soln. was filtered and cooled to obtain 156 g. Me 2-nitro-4-methyldiphenyl sulfide-2'-carboxylate, m. 140-6.degree.. This compd. (150 g.) gave on hydrogenation in 1100 cc. EtOAc in the presence of 70 g. Ni catalyst 125 g. Me 2-amino-4-methyldiphenyl sulfide-2'-carboxylate, m. 83-5.degree., 60 g. of which was heated at 240-70.degree. for 1 hr., while MeOH was distd. and 40 min. at that temp. in vacuo. After cooling the residue was extd. with 50 cc. anhyd. alc. and filtered to obtain 47 g. II (R2= Me, R = R1 = R3 = H) (III), m. 288-91.degree. (AcOH). A soln. of 28 g. III and 6.4 g. NaNH2 in 300 cc. dioxane was heated 3 hrs. until no more NH3 was formed. After cooling to 60.degree. the stirred mixt. was treated with 22.4 g. .beta.-dimethylaminoethyl chloride in 60 cc. anhyd. benzene within 30 min. and the mixt. refluxed 3 hrs. After filtration of NaCl the filtrate was evapd. in vacuo, the residue dissolved in 200 cc. Et2O, and extd. with dil. HCl. The acid ext. was made alk., the base dissolved in Et2O, dried, and the solvent evapd. to obtain 33 g. II (R2 = Me, R3 = Me2NCH2CH2, R = R1 = H) (IV), m. 109-10.degree. (iso-PrOH-petr. ether), the antihistaminic effect of which was 3 times as great as that of 10-(.beta.-dimethylaminoethyl)phenothiazine in a test on guinea pigs according to the method of Kallos and Pagel. The HCl salt of IV, m. 223-5.degree., was prepd. in EtOAc. The following II were also prepd. (R, R1, R2, R3, % yield, m.p., and m.p. HCl salt given): H, H, Me, iso-PrMeNCH2CH2, 85, 92-3.degree., 209-10.degree.; H, H, Me, Et2NCH2CH2, 72-3.degree., 197-9.degree.; H, H, Me, Me2N(CH2)3, 92, 83-5.degree., 170-2.degree.; H, Me, H, H, -, 272-4.degree., -, H, Me, H, Me2NCH2CH2, 90, 75-6.degree., 236-7.degree.; Me, H, H, H, -, 257-8.degree., -, H, Me, Me, H, -, 303-5.degree., -, H, H, MeO, H, -, 218-19.degree., -, Me, H, H, Me2NCH2CH2, 87, 105-7.degree., 240-1.degree.; H, Me, Me, Me2NCH2CH2, 90, 114-15.degree., 255-7.degree. (decompn.); H, H, MeO, Me2NCH2CH2, -, - (oil), 189-92.degree.; H, H, MeO, Et2NCH2CH2, -, - (oil), 190-2.degree.; H, H, MeO, Me2N(CH2)3, -, 104-6.degree., 141-3.degree.. The following substituted 2'-carbomethoxydiphenyl sulfides were prepd. (substituents and

m.p. given): 2-O₂N, 5-Me, 86-8.degree.; 2-H₂N, 5-Me, 82-4.degree.; 2-O₂N, 6-Me, 100-2.degree.; 2-H₂N, 6-Me, 86-7.degree.; 2-O₂N, 4,5-Me₂, 93-5.degree.; 2-H₂N, 4,5-Me₂, 130-2.degree.; 2-O₂N, 4-MeO, 105-6.degree.; 2-H₂N, 4-MeO, 134-5.degree..

IT 3159-07-7, Dibenzo[b,f][1,4]thiazepin-11(10H)-one
(derivs.)

RN 3159-07-7 CAPLUS

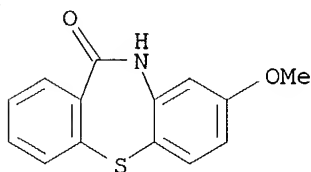
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 3159-05-5, Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methoxy-
29308-82-5, Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methyl-
88112-09-8, Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 7-methyl-
96953-80-9, Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 6-methyl-
97213-14-4, Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 7,8-dimethyl-
100726-00-9, Benzoic acid, o-(2-nitro-p-tolylthio)-
(prepn. of)

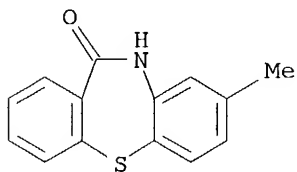
RN 3159-05-5 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methoxy- (6CI, 7CI, 8CI, 9CI)
(CA INDEX NAME)



RN 29308-82-5 CAPLUS

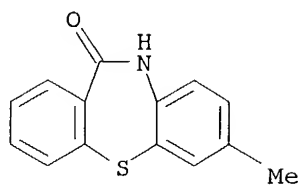
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 8-methyl- (6CI, 7CI, 8CI) (CA INDEX NAME)



RN 88112-09-8 CAPLUS

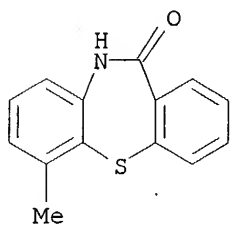
CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 7-methyl- (6CI, 9CI) (CA INDEX NAME)

10/030,251



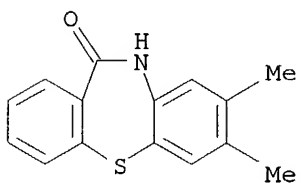
RN 96953-80-9 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 6-methyl- (6CI, 7CI) (CA INDEX NAME)



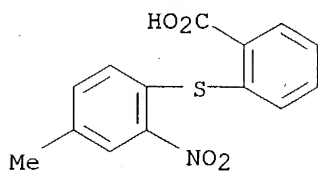
RN 97213-14-4 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 7,8-dimethyl- (6CI, 7CI) (CA INDEX NAME)



RN 100726-00-9 CAPLUS

CN Benzoic acid, o-(2-nitro-p-tolylthio)- (6CI) (CA INDEX NAME)



~~IX~~3 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1958:25574 CAPLUS

DOCUMENT NUMBER: 52:25574

ORIGINAL REFERENCE NO.: 52:4652e-i,4653a-c

TITLE: Antihistamine substances. XLIII. Derivatives of
1-aza-4-thia-2,3,5,6-dibenzocycloheptadiene
(homophenothiazine)

AUTHOR(S): Hach, Vladimir; Protiva, Miroslav

CORPORATE SOURCE: Pharm. and Biochem. Research Inst., Prague

SOURCE: Chemicke Listy pro Vedu a Prumysl (1957), 51, 1909-14
CODEN: CLPRAN; ISSN: 0366-6832

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 51, 17944a. The authors propose for I (R = H) the name hemophenothiazine and the given numbering system. Adding to MeONa (from 19.0 g. Na and 500 ml. MeOH) 98 g. .omicron.-MeO₂CC₆H₄SH then under stirring and ice-cooling 92.2 g. .omicron.-ClC₆H₄NO₂, heating the mixt. at 50.degree. 15 hrs. under stirring, cooling, combining the sepd. product with the ppt. obtained by dilg. the filtrate with H₂O and recrystg. from MeOH gave 94 g. crude Me ester of 2-O₂NC₆H₄SC₆H₄CO₂H-2 (II); pure II m. 92-3.degree.. II (13.8 g.) hydrogenated over PtO₂ in 150 ml. 96% EtOH gave the Me ester of 2-H₂NC₆H₄SC₆H₄CO₂H-2 (III), m. 95-6.degree. (75% EtOH). III (20.0 g.) heated in an oil bath 7 hrs. to 200-20.degree. and the solidified molten mass recrystd. (aq. EtOH) gave the lactam (IV) of III, 15.0 g., m. 239-42.degree. (aq. EtOH). Refluxing 30 hrs. a mixt. of 12.0 g. IV, 3.0 g. LiAlH₄, and 500 ml. abs. Et₂O, cooling, decomp. the mixt. with 35 ml. 10% NaOH, extg. the aq. layer with Et₂O, combining the Et₂O solns., and evapg. the Et₂O gave 10.0 g. I (R = H), m. 115.degree. (EtOH); hydrochloride, m. 175.degree. (EtOH-Et₂O). Refluxing 50 ml. of abs. xylene, 7.1 g. I (R = H), 1.9 g. finely ground NaNH₂, and 5.5 g. Cl(CH₂)₂NMe₂ 10 hrs. in an oil bath, cooling, decomp. the mixt. with 20 ml. H₂O, extg. the base with 100 ml. 10% HCl, filtering, extg. the alkalized soln. with C₆H₆, and evapg. C₆H₆ gave, on distn., 6.4 g. I [R = (CH₂)₂NMe₂], b0.5 160-5.degree.; hydrochloride, m. 206.degree. (EtOH-Et₂O); picrate, m. 156.degree. (EtOH); methiodide, m. 195.degree. (EtOH-Et₂O). By an analogous procedure were obtained: N-(2-piperidino-ethyl)homophenothiazine, b0.5 180.degree. [acid succinate, m. 150-1.degree., (EtOH); picrate, m. 165.degree. (EtOH)]; I (R = CH₂CH-MeNMe₂), b0.5 165-70.degree., 68% [picrate, m. 158.degree. (EtOH)]; I [R = (CH₂)₃NMe₂], b0.5 169-73.degree., 67% [hydrobromide, m. 157.degree.; picrate, m. 135.degree. (EtOH)]. Refluxing 10.5 g. I (R = H), 8.0 g. ClCH₂COCl, and 100 ml. C₆H₆ 3 hrs. to 80.degree. gave 11.0 g. I (R = COCH₂Cl), m. 103.degree. (EtOH); refluxing the preceding compd. (9.3 g.) with 14 mg. NH₄Et and 120 ml. C₆H₆ gave 7.8 g. I (R = COCH₂NEt₂), b0.6 190-5.degree., m. 51-3.degree. (petr. ether); picrate, m. 175.degree. (EtOH); ethobromide, m. 188.degree. (decompn.) (EtOH-Et₂O). Refluxing 5.0 g. I [R = CO(CH₂)₂Cl], m. 98.degree. (EtOH), obtained as above, with 4.0 g. dry MeSNa and 100 ml. abs. Me₂CO 6 hrs. on an H₂O bath, evapg. the Me₂CO, dilg. the residue with H₂O, and extg. with C₆H₆ yielded, on distn., 3.8 g. crude sulfide, b0.8 175-80.degree., which gave, after standing with 15 ml. MeI, I [R = CO(CH₂)₂S(+)Me₂I(-)], m. 133.degree. (decompn.) (EtOH-Et₂O). The aminoalkyl derivs. of I are very effective antihistaminics and local anesthetics. The quaternary salts are less effective and practically without local anesthetic effect, but show an antispasmodic activity.

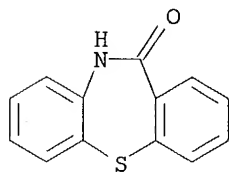
IT 3159-07-7, Dibenzo[b,f][1,4]thiazepin-11(10H)-one
19806-43-0, Benzoic acid, o-(o-nitrophenylthio)-

10/030,251

(prepn. of)

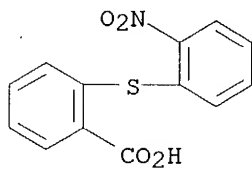
RN 3159-07-7 CAPLUS

CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 19806-43-0 CAPLUS

CN Benzoic acid, 2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



12813

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1958:25574 CAPLUS
 DOCUMENT NUMBER: 52:25574
 ORIGINAL REFERENCE NO.: 52:4652e-i,4653a-c
 TITLE: Antihistamine substances. XLII. Derivatives of
 1-aza-4-thia-2,3,5,6-dibenzocycloheptadiene
 (homophenothiazine)
 AUTHOR(S): Hach, Vladimir; Protiva, Miroslav
 CORPORATE SOURCE: Pharm. and Biochem. Research Inst., Prague
 SOURCE: Chemicke Listy pro Vedu a Prumysl (1957), 51, 1909-14
 CODEN: CLPRAN; ISSN: 0366-6832
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 51, 17944a. The authors propose for I (R = H) the name
 hemophenothiazine and the given numbering system. Adding to MeONa (from
 19.0 g. Na and 500 ml. MeOH) 98 g. o-MeO₂CC₆H₄SH then under
 stirring and ice-cooling 92.2 g. o-ClC₆H₄NO₂, heating the mixture at
 50° 15 hrs. under stirring, cooling, combining the separated product
 with the precipitate obtained by diluting the filtrate with H₂O and recrystg.

from

MeOH gave 94 g. crude Me ester of 2-O₂NC₆H₄SC₆H₄CO₂H-2 (II); pure II m.
 92-3°. II (13.8 g.) hydrogenated over PtO₂ in 150 ml. 96% EtOH
 gave the Me ester of 2-H₂NC₆H₄SC₆H₄CO₂H-2 (III), m. 95-6° (75%
 EtOH). III (20.0 g.) heated in an oil bath 7 hrs. to 200-20° and
 the solidified molten mass recrystd. (aqueous EtOH) gave the lactam (IV) of
 III, 15.0 g., m. 239-42° (aqueous EtOH). Refluxing 30 hrs. a mixture of
 12.0 g. IV, 3.0 g. LiAlH₄, and 500 ml. absolute Et₂O, cooling, decomposing the
 mixture with 35 ml. 10% NaOH, extracting the aqueous layer with Et₂O,

combining the

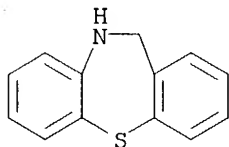
Et₂O solns., and evaporating the Et₂O gave 10.0 g. I (R = H), m. 115°
 (EtOH); hydrochloride, m. 175° (EtOH-Et₂O). Refluxing 50 ml. of
 absolute xylene, 7.1 g. I (R = H), 1.9 g. finely ground NaNH₂, and 5.5 g.
 Cl(CH₂)₂NMe₂ 10 hrs. in an oil bath, cooling, decomposing the mixture with 20
 ml. H₂O, extracting the base with 100 ml. 10% HCl, filtering, extracting the
 alkalized solution with C₆H₆, and evaporating C₆H₆ gave, on distillation, 6.4

g. I [R =

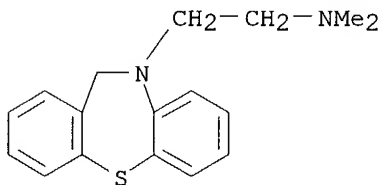
(CH₂)₂NMe₂], b0.5 160-5°; hydrochloride, m. 206°
 (EtOH-Et₂O); picrate, m. 156° (EtOH); methiodide, m. 195°
 (EtOH-Et₂O). By an analogous procedure were obtained:
 N-(2-piperidino-ethyl)homophenothiazine, b0.5 180° [acid succinate,
 m. 150-1°, (EtOH); picrate, m. 165° (EtOH)]; I (R =
 CH₂CH-MeNMe₂), b0.5 165-70°, 68% [picrate, m. 158° (EtOH)];
 I [R = (CH₂)₃NMe₂], b0.5 169-73°, 67% [hydrobromide, m.
 157°; picrate, m. 135° (EtOH)]. Refluxing 10.5 g. I (R =
 H), 8.0 g. ClCH₂COCl, and 100 ml. C₆H₆ 3 hrs. to 80° gave 11.0 g. I
 (R = COCH₂Cl), m. 103° (EtOH); refluxing the preceding compound (9.3
 g.) with 14 mg. NH₄Et and 120 ml. C₆H₆ gave 7.8 g. I (R = COCH₂NEt₂), b0.6
 190-5°, m. 51-3° (petr. ether); picrate, m. 175°
 (EtOH); ethobromide, m. 188° (decomposition) (EtOH-Et₂O). Refluxing 5.0
 g. I [R = CO(CH₂)₂Cl], m. 98° (EtOH), obtained as above, with 4.0
 g. dry MeSNa and 100 ml. absolute Me₂CO 6 hrs. on an H₂O bath, evaporating the
 Me₂CO, diluting the residue with H₂O, and extracting with C₆H₆ yielded, on
 distillation,

3.8 g. crude sulfide, b0.8 175-80°, which gave, after standing with
 15 ml. MeI, I [R = CO(CH₂)₂S(+)Me₂I(-)], m. 133° (decomposition)
 (EtOH-Et₂O). The aminoalkyl derivs. of I are very effective
 antihistaminics and local anesthetics. The quaternary salts are less
 effective and practically without local anesthetic effect, but show an
 antispasmodic activity.

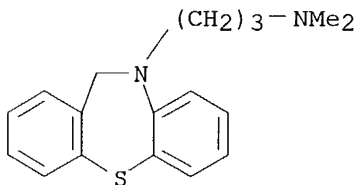
IT 494-20-2, Dibenzo[b,f][1,4]thiazepine, 10,11-dihydro-
 6768-40-7, Dibenzo[b,f][1,4]thiazepine, 10-(2-dimethylaminoethyl)-
 10,11-dihydro- 6768-42-9, Dibenzo[b,f][1,4]thiazepine,
 10-[3-dimethylaminopropyl]-10,11-dihydro- 54920-98-8, Benzoic
 acid, o-(o-aminophenylthio)- 112626-08-1,
 Dibenzo[b,f][1,4]thiazepine, 10,11-dihydro-10-(2-piperidinoethyl)-
 113010-99-4, Dibenzo[b,f][1,4]thiazepine, 10-(N,N-diethylglycyl)-
 10,11-dihydro-
 (and derivs.)
 RN 494-20-2 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepine, 10,11-dihydro- (6CI, 7CI, 8CI, 9CI) (CA
 INDEX NAME)



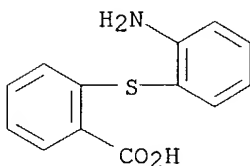
RN 6768-40-7 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepine, 10-[2-(dimethylamino)ethyl]-10,11-dihydro-
 (6CI, 7CI, 8CI) (CA INDEX NAME)



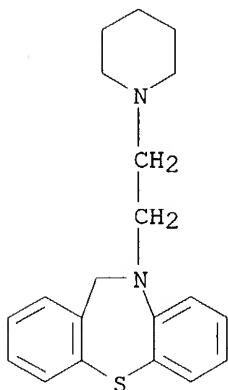
RN 6768-42-9 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepine, 10-[3-(dimethylamino)propyl]-10,11-dihydro-
 (6CI, 7CI, 8CI) (CA INDEX NAME)



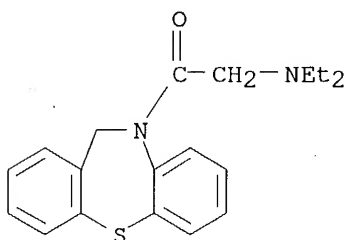
RN 54920-98-8 CAPLUS
 CN Benzoic acid, 2-[(2-aminophenyl)thio]- (9CI) (CA INDEX NAME)



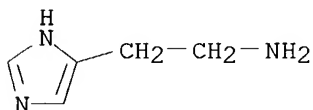
RN 112626-08-1 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepine, 10,11-dihydro-10-(2-piperidinoethyl)- (6CI)
 (CA INDEX NAME)



RN 113010-99-4 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepine, 10-(N,N-diethylglycyl)-10,11-dihydro- (6CI)
 (CA INDEX NAME)

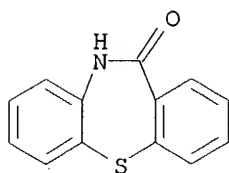


IT **51-45-6**, Histamine
 (antihistamine substances)
 RN 51-45-6 CAPLUS
 CN 1H-Imidazole-4-ethanamine (9CI) (CA INDEX NAME)



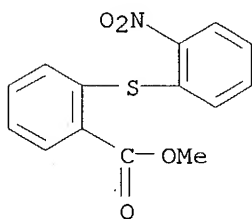
IT **3159-07-7**, Dibenzo[b,f][1,4]thiazepin-11(10H)-one
4892-03-9, Benzoic acid, o-(o-nitrophenylthio)-, methyl ester
19806-43-0, Benzoic acid, o-(o-nitrophenylthio)-
109257-21-8, Dibenzo[b,f][1,4]thiazepine, 10-chloroacetyl-10,11-dihydro-
110178-46-6, Dibenzo[b,f][1,4]thiazepine, 10,11-dihydro-10-[3-(methylthio)propionyl]-
130831-20-8, Dibenzo[b,f][1,4]thiazepine, 10-(3-chloropropionyl)-10,11-dihydro-
 (preparation of)
 RN 3159-07-7 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

NAME)



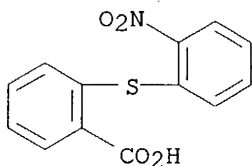
RN 4892-03-9 CAPLUS

CN Benzoic acid, 2-[(2-nitrophenyl)thio]-, methyl ester (9CI) (CA INDEX NAME)



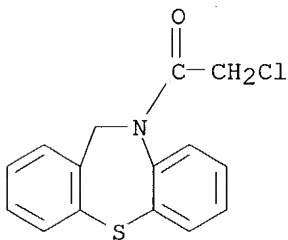
RN 19806-43-0 CAPLUS

CN Benzoic acid, 2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



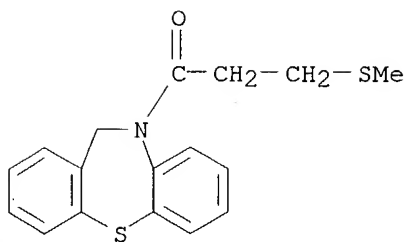
RN 109257-21-8 CAPLUS

CN Dibenzo[b,f][1,4]thiazepine, 10-chloroacetyl-10,11-dihydro- (6CI) (CA INDEX NAME)



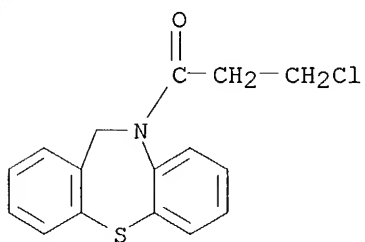
RN 110178-46-6 CAPLUS

CN Dibenzo[b,f][1,4]thiazepine, 10,11-dihydro-10-[3-(methylthio)propionyl]- (6CI) (CA INDEX NAME)



RN 130831-20-8 CAPLUS

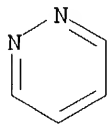
CN Dibenzo[b,f][1,4]thiazepine, 10-(3-chloropropionyl)-10,11-dihydro- (6CI)
(CA INDEX NAME)



IT 289-80-5, Pyridazine
(quaternary derivs.)

RN 289-80-5 CAPLUS

CN Pyridazine (8CI, 9CI) (CA INDEX NAME)



ANSWER 13 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1958:11111 CAPLUS

DOCUMENT NUMBER: 52:11111

ORIGINAL REFERENCE NO.: 52:2004c-i,2005a-b

TITLE: Beckmann rearrangement of some cyclic sulfone ketoximes

AUTHOR(S): Truce, W. E.; Simms, J. A.

CORPORATE SOURCE: Purdue Univ., Lafayette, IN

SOURCE: Journal of Organic Chemistry (1957), 22, 617-20

CODEN: JOCEAH; ISSN: 0022-3263

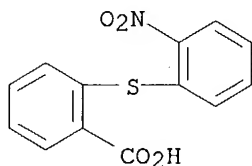
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

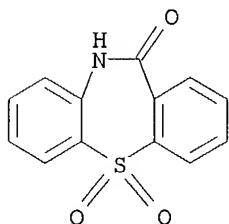
AB The ease of rearrangement of 10-thiaxanthenone 5,5-dioxide oxime (I), 4-thiachromanone 1,1-dioxide oxime (II), and tetrahydro-4H-1-thiapyran-4-one 1,1-dioxide oxime (III) was found to be III mchgt. II equal or nearly equal to I. The rearrangement product of I was characterized by independent synthesis. C₆H₆ and .omicron.-HSC₆H₄CO₂H (IIIIa) gave 68% 10-thiaxanthenone (IV), m. 213-14.degree.. IV with H₂O₂ in AcOH according to Ullmann and von Glenck (C.A. 11, 2668) gave a quant. yield of the 5,5-dioxide (V), m. 187-8.5.degree.. V (10 g.), 16 g. H₂NOH.HCl, and 30 ml. C₅H₅N in 150 ml. alc. refluxed 23 hrs. gave 9.6 g. I, m. 213-14.degree.; shorter reaction times produced a mixt. contg. unreacted V. PC15 (10.2 g.) in 75 ml. POCl₃ refluxed 48 hrs. with 9 g. I in 125 ml. POCl₃, the solvent removed, the residue poured into ice H₂O, extd. with Et₂O, distd., the residue heated 1 hr. with 300 ml. 50% H₂SO₄, and the product (8.1 g.) heated 1.5 hrs. with 300 ml. 7% NaOH gave 0.9 g. V and 3 fractions: (1) 1.1 g., m. 291-2.5.degree.; (2) 1.5 g., m. 289-91.degree.; (3) 1.7 g., m. 289.5-90.degree.. A mixt. of 1 and 2-(2-H₂NC₆H₄SO₂)C₆H₄CO₂H (VI) gave no depression. The yield of VI dropped with a reflux time of 16 hrs., and more V was isolated. A 3-step synthesis, starting with IIIa and .omicron.-O₂NC₆H₄Cl, gave a low yield of VI. IIIa (50 g.) and 15 g. Na in 300 ml. alc. refluxed 4 hrs. with 51 g. .omicron.-O₂NC₆H₄Cl in 300 ml. alc. gave 28.8 g. 2-(2-HO₂CC₆H₄S)C₆H₄NO₂ (VII), m. 166-9.degree.. VII (24 g.) in 200 ml. AcOH treated with 29 ml. 30% H₂O₂ at such a rate as to maintain gentle reflux, and the mixt. refluxed 3 hrs. and concd. gave 21.5 g. 2-(2-O₂NC₆H₄SO₂)C₆H₄CO₂H (VIII), m. 198-200.degree.. VIII (10 g.) suspended in 200 ml. concd. HCl treated under reflux with 23.7 g. Sn, heated 3 hrs. on a steam bath, and the product pptd. by cooling gave 6.7 g. crude VI, m. 287-8.degree. (alc.-AcOH); during drying VI evidently cyclized to the corresponding lactam. Cl(CH₂)₂CO₂H and PhSH gave 83% PhSCH₂CH₂CO₂H (IX). IX gave 68% 4-thiachromanone (X), oxidized with H₂O₂ in AcOH to 64% of the 1,1-dioxide (XI), m. 128-9.5.degree.. XI (20 g.) similarly treated with H₂NOH.HCl in C₅H₅N and alc. gave 19.1 g. II, m. 193.5-4.5.degree. (from H₂O). None of the expected rearrangement product, the lactam (XIa) of 2-H₂NC₆H₄CH₂CH₂CO₂H, was isolated in any of a series of 7 expts. The catalysts, PC15, 85% H₂SO₄, 93% H₂SO₄, and polyphosphoric acid, caused tar formation or hydrolysis to XI. In a no. of cases II was recovered. II was very resistant to hydrolysis or rearrangement when heated with concd. H₂SO₄. The solvents used for the 7 expts. in order were: POCl₃, Et₂O, Et₂O, CHCl₃, 85% H₂SO₄, 93% H₂SO₄, and polyphosphoric acid. II (6.33 g.) with 225 ml. H₂O and 5.55 g. PhSO₂Cl left 19 hrs. at room temp. with 33 ml. N NaOH and refluxed 1 hr. gave 6.05 g. II N-benzenesulfonate (XII), m. 150.5-1.0.degree. (Et₂O-CHCl₃). XII did not rearrange when heated 0.5 hr. at 140.degree. with polyphosphoric acid; the product contained 20% starting material and tar. XII was recovered quantitatively when heated 6 hrs. at 100.degree. in MeOH in a sealed tube. Concd. HCl 3 hrs. at 120.degree. gave only tar. II (2.10 g.) and 2.33 g. .omicron.-

O₂NC₆H₄SO₂Cl yielded 3.52 g. of II .omicron.-nitrobenzenesulfonate (XIII), m. 182.5.degree. (decompn.) (dioxane-H₂O). XIII (0.90 g.) heated 12 hrs. at 120.degree. with 40 ml. concd. HCl in a sealed tube gave 0.21 g. XIa, m. 243-4.degree. (in alc. pptd. by Et₂O). S(CH₂CH₂CO₂Me)₂ gave 10% tetrahydro-4H-1-thiapyranone, m. 60-3.degree., oxidized with 30% H₂O₂ to the 1,1-dioxide (XIV), m. 171.degree.. XIV (3.6 g.), 2.1 g. H₂NOH.HCl, and 2.6 g. Na₂CO₃ in 150 ml. H₂O refluxed, then kept 11 hrs., and the solid extd. in a Soxhlet app. gave 1.57 g. III, m. 197-201.degree.. III (1.5 g.) heated 2 min. with 12 ml. 85% H₂SO₄ gave 1.76 g. MeOH-sol., infusible material, probably H₂NCH₂CH₂SO₃K. The mechanism of the above reactions is discussed.

IT 19806-43-0, Benzoic acid, o-(o-nitrophenylthio)-
 22871-33-6, Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 5,5-dioxide
 99847-56-0, Benzoic acid, o-(o-nitrophenylsulfonyl)-
 (prepn. of)
 RN 19806-43-0 CAPLUS
 CN Benzoic acid, 2-[(2-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



RN 22871-33-6 CAPLUS
 CN Dibenzo[b,f][1,4]thiazepin-11(10H)-one, 5,5-dioxide (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 99847-56-0 CAPLUS
 CN Benzoic acid, o-(o-nitrophenylsulfonyl)- (6CI) (CA INDEX NAME)

